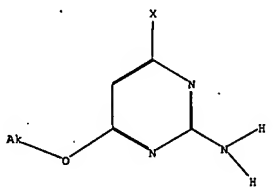
EAST Search History

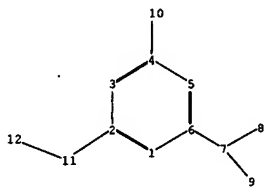
Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	825	(544/320).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:41
L2	460	(544/334).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:41
L3	49	Sylvia.inv. and Huber.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:40
L4	0	Thomas.inv. and Gutner.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:41
L5	11	Thomas.inv. and Guthner.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:41
L6	136	Wolfgang.inv. and Moser.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:42
L7	9	Doris.inv. and Krammer.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:42

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	825	(544/320).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:41
L2	460	(544/334).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:41
L3	49	Sylvia.inv. and Huber.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:40
L4	0	Thomas.inv. and Gutner.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:41
L5	11	Thomas.inv. and Guthner.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:41
L6	136	Wolfgang.inv. and Moser.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:42
L7	9	Doris.inv. and Krammer.inv.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/06/19 15:42

C:\Program Files\Stnexp\Queries\10528959.str





chain nodes :
7 8 9 10 11 12
ring nodes :
1 2 3 4 5 6
chain bonds :
2-11 4-10 6-7 7-8 7-9 11-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-11 6-7 11-12
exact bonds :
4-10 7-8 7-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Connectivity :
12:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS

10/528,959

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NEWS 4	MAR 20	MARPAT now updated daily
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NEWS 6	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 7	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 8	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 9	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 10	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 11	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 12	MAY 01	New CAS web site launched
NEWS 13	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 14	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 15	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 16	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 17	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 18	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 19	JUN 18	CA/CAplus to be enhanced with pre-1967 CAS Registry Numbers

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:07:52 ON 19 JUN 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:08:04 ON 19 JUN 2007

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 JUN 2007 HIGHEST RN 937778-45-5
DICTIONARY FILE UPDATES: 18 JUN 2007 HIGHEST RN 937778-45-5

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http://www.cas.org/support/stngen/stndoc/properties.html

=>
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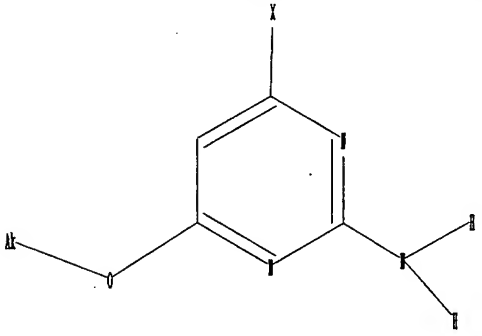

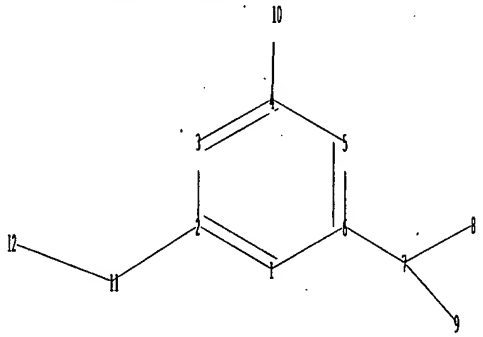

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ring nodes :
1 2 3 4 5 6
chain bonds :
2-11 4-10 6-7 7-8 7-9 11-12
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2-11 6-7 11-12
exact bonds :
4-10 7-8 7-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Connectivity :
12:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

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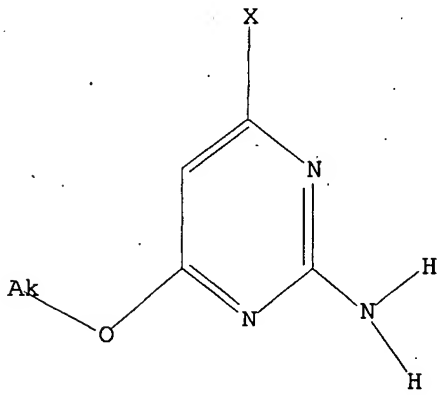
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
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SAMPLE SCREEN SEARCH COMPLETED - 141 TO ITERATE

100.0% PROCESSED 141 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

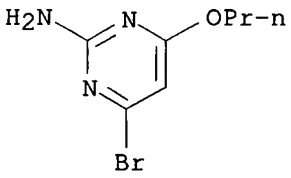
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2108 TO 3532
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> d scan

10/528,959

L2 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Pyrimidinamine, 4-bromo-6-propoxy- (9CI)
MF C7 H10 Br N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

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FULL SCREEN SEARCH COMPLETED -     2663 TO ITERATE

100.0% PROCESSED     2663 ITERATIONS                          36 ANSWERS
SEARCH TIME: 00.00.01

L3           36 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               172.10     172.31

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FILE LAST UPDATED: 18 Jun 2007  (20070618/ED)

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=> s l3
L4          126 L3

=> s l4/prep
FIELD CODES CANNOT BE CHANGED HERE
You may have tried to apply a field code to a term that already has a
field code.  You can only add a field code to a term that has no field
code appended to it.

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        4419395 PREP/RL
L5           34 L3/PREP
                   (L3 (L) PREP/RL)

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L5 ANSWER 1 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:1263576 CAPLUS
DN 144:128931
TI Synthesis of N-aryl-2-amino-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidine-6-carboxamides
AU Tumkevicius, S.; Dailide, M.
CS Department of Organic Chemistry, Faculty of Chemistry, Vilnius University, Vilnius, LT-03225, Lithuania
SO Journal of Heterocyclic Chemistry (2005), 42(7), 1305-1310
CODEN: JHTCAD; ISSN: 0022-152X
PB HeteroCorporation
DT Journal
LA English
OS CASREACT 144:128931
AB Synthetic routes for the preparation of Me 2-amino-4-(methoxy)thieno[2,3-d]pyrimidine-6-carboxylate (I) (a useful intermediate for lipophilic and classical antifolates) from 2-amino-4,6-dichloro-5-pyrimidinecarboxaldehyde have been studied. It has been shown that more efficient synthesis of I includes the preparation of a 4-methoxy derivative and subsequent tandem substitution/annulation reaction with Me mercaptoacetate in DMF in the presence of potassium carbonate and mol. sieves 4A. I was used for the synthesis of N-aryl-2-amino-4-oxo-3,4-dihydrothieno[2,3-d]-pyrimidine-6-carboxamide derivs., including an analog of folic acid with amide bridge [i.e., N-(4-{[(2-amino-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-6-yl)carbonyl]amino}-benzoyl)-L-glutamic acid].
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:554169 CAPLUS
DN 144:331376
TI Synthesis of 2-(pyrimidin-2-yl)amino-4H-pyrido[3,2-e][1,3]thiazin-4-one derivatives in one port reaction method
AU Sun, Xiao-Hong; Ji, Peng-Ju; Liu, Yuan-Fa; Chen, Bang; Jia, Ying-Qi
CS Institute of Chemistry, Northwest University, Xi'an, 710069, Peop. Rep. China
SO Youji Huaxue (2005), 25(6), 724-726
CODEN: YCHHDX; ISSN: 0253-2786
PB Youji Huaxue Bianjibu
DT Journal
LA Chinese
OS CASREACT 144:331376
AB 2-Chloronicotioyl isothiocyanate reacted with substituted 2-aminopyrimidine under the alkali condition to give 2-(pyrimidin-2-yl)amino-4H-pyrido[3,2-e][1,3]thiazin-4-one directly. Six 2-(pyrimidin-2-yl)amino-4H-pyrido[3,2-e][1,3]thiazin-4-one compds. were synthesized. The structures of these compds. were confirmed by IR, 1H NMR spectra and elemental analyses. A possible mechanism of the reaction was proposed.

L5 ANSWER 3 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:370910 CAPLUS
DN 140:375181
TI Etherification method for the production of 2-amino-4-chloro-6-alkoxypyrimidines from 2-amino-4,6-dichloropyrimidine and alkali metal alkoxides or alkali and alkanols
IN Huber, Sylvia; Guethner, Thomas; Moser, Wolfgang; Krammer, Doris
PA Degussa A.-G., Germany
SO PCT Int. Appl., 16 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004037795	A1	20040506	WO 2003-EP11844	20031024
	W: JP, US				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
	DE 10249946	A1	20040519	DE 2002-10249946	20021026
	DE 10249946	B4	20050623		
	EP 1554255	A1	20050720	EP 2003-775230	20031024
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
	JP 2006512305	T	20060413	JP 2004-545989	20031024
	US 2006035913	A1	20060216	US 2005-528959	20050322
PRAI	DE 2002-10249946	A	20021026		
	WO 2003-EP11844	W	20031024		

OS CASREACT 140:375181
AB 2-Amino-4-chloro-6-alkoxypyrimidines (e.g., 2-amino-4-chloro-6-methoxypyrimidine) are prepared in high yield and selectivity by reacting 2-amino-4,6-dichloropyrimidine with an alkali metal alcoholate (e.g., sodium methoxide) or a mixture of alkali hydroxides and an alc. in a polar aprotic solvent (e.g., acetone), or a solvent mixture, where the solvent is distilled off to >30% percent and the product is precipitated by adding water during or following the distillation process.
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:205964 CAPLUS
DN 142:74474
TI Product class 12: pyrimidines
AU von Angerer, S.
CS Germany
SO Science of Synthesis (2004), 16, 379-572
CODEN: SSCYJ9
PB Georg Thieme Verlag
DT Journal; General Review
LA English
AB A review. Methods for preparing pyrimidines are reviewed including cyclization, ring transformation, aromatization and substituent modification.
RE.CNT 856 THERE ARE 856 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:857826 CAPLUS
DN 137:321562
TI Sulfonyl urea compound and its application as a herbicide
IN Zhao, Fengge; Cao, Guanghong; Xie, Longguan; Jiang, Jun; Cheng, Muru; Lu, Qingsong; Han, Yimin; Ye, Hongyu; Chen, Xiaohui
PA Lianyungang City No.2 Pesticide Plant, Peop. Rep. China
SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 9 pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CN 1337158	A	20020227	CN 2000-112466	20000815
PRAI	CN 2000-112466		20000815		

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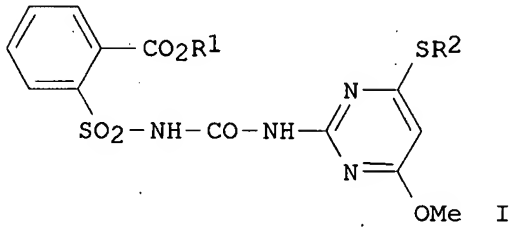
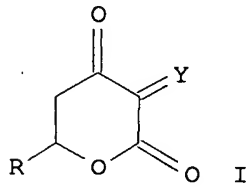


I

AB Sulfonyl urea compds. I (where: R1 = Me, Et, or iso-Pr and R2 = alkyl, alkenyl, heterocyclic group, aryl, alkylheterocyclic group, or arylalkyl) are synthesized by substituting 4,6-dichloro-2-pyrimidinamine with Na methoxide, substituting again with NaHS and acidifying to obtain 2-amino-6-methoxy-4-pyrimidinethiol;S-alkylating with R2X to obtain 4-(R2S)-6-methoxy-2-pyrimidinethiol (a); allowing to react 2-(R1O-carbonyl)phenylsulfonamide with oxalyl chloride to obtain 2-(R1O-carbonyl)phenylsulfonyl isocyanate (b); and then condensing (a) with (b). The sulfonyl urea compds. may be used as herbicides.

L5 ANSWER 6 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:610319 CAPLUS
DN 135:344347
TI Synthesis and fungicidal activity of 3-heterocyclylaminomethylene-5,6-dihydro-6-alkyl(aryl)-2H-pyran-2,4-diones
AU Wang, You-Ming; Li, Zheng-Ming; Han, Yu-Fen; Jia, Bao-Jun; Wang, Yu-Lin
CS Institute of Elemento-Organic Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China
SO Yingyong Huaxue (2001), 18(7), 524-527
CODEN: YIHUED; ISSN: 1000-0518
PB Yingyong Huaxue Bianji Weiyuanhui
DT Journal
LA Chinese
OS CASREACT 135:344347
GI



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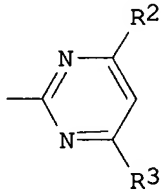
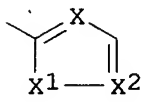
Q = 

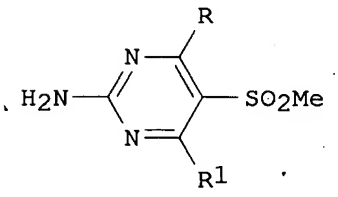
Q1 = 

AB Title compds. I (R = CH3(CH2)2, C6H5; Y = CHNHR1; R1 = Q, Q1; R2 = CH3O, CH3, H, Cl; R3 = H, CH3O, CH3; X = N, CCN, CCOOEt; X1 = S, NCH3, NC6H5; X2 = CH, N) were prepared by condensation of I (Y = H2) with Et orthoformate and R1NH2. A pair of conformational isomers existed in I due to the intramol. hydrogen bonding. Title compds. I were tested in vitro against H. Oryzae, B. Cinerae and S. Sclerotiorum, showing some fungicidal activity.

L5 ANSWER 7 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:703333 CAPLUS
DN 134:162984
TI Synthesis of 2-amino-4-chloro-6-methoxypyrimidine
AU Zhu, Lu; Zhao, Lei; Ren, Cui-ping
CS School of Chemistry and Chemical Engineering, Zhengzhou University, Zhengzhou, 450052, Peop. Rep. China
SO Zhengzhou Daxue Xuebao, Ziran Kexueban (2000), 32(2), 87-88
CODEN: ZDZKFG; ISSN: 1001-8212
PB Zhengzhou Daxue Xuebao Bianjibu
DT Journal
LA Chinese
OS CASREACT 134:162984
AB Guanidine nitrate and di-Et malonate were used to synthesis 2-amino-4-chloro-6-methoxypyrimidine, by cyclization, chloridization hydrolysis and methoxylation. The yield reaches 70% and the structure is confirmed by IR test. The goal compound, 2-amino-4-chloro-6-methoxypyrimidine, is a key intermediate for preparing anticancer medicine.

L5 ANSWER 8 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:211315 CAPLUS
DN 132:308038
TI Capillary electrochromatography of pyrimidine derivatives using UV and mass spectrometric detection
AU Ahrer, Werner; Hagenauer, Isolde; Buchberger, Wolfgang
CS Department of Analytical Chemistry, University of Linz, Linz, A-4040, Austria
SO Monatshefte fuer Chemie (2000), 131(2), 155-163
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer-Verlag Wien
DT Journal
LA English
AB The separation of pyrimidine derivs. by capillary electrochromatog. (CEC) using either UV or mass spectrometric detection is described. For UV detection an aqueous phosphate carrier electrolyte containing MeCN is employed. The results are compared to the anal. of the same compds. by micellar electrokinetic chromatog. in terms of selectivity, migration times, linearity, and detection limits. For the combination of CEC and mass spectrometry (MS) an inexpensive way to couple com. available instruments is presented; the interface consists of an elec. grounded stainless steel connector (containing a stainless steel frit) serving as the electrode and coupling the CEC capillary with a fused SiO2 transfer capillary to the MS instrument. Alternatively, a PEEK adapter combining the CEC capillary and a grounded stainless steel transfer capillary serving as the electrode is employed. To avoid the formation of H gas at the coupling piece or the transfer capillary, p-benzoquinone is added to the carrier electrolyte consisting of aqueous NH4OAc and MeCN.
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:874233 CAPLUS
DN 124:86931
TI Synthesis of new 2-amino-4-cyanomethyl-5-methylsulfonylpyrimidine derivatives
AU Kim, Jung-Hwan; Han, Mun-Su; Kim, Un-Ju
CS Dep. Chem., Yeungnam Univ., Gyongsan, 712-749, S. Korea
SO Journal of the Korean Chemical Society (1995), 39(9), 728-33
CODEN: JKCSEZ; ISSN: 1017-2548
PB Korean Chemical Society
DT Journal
LA Korean
GI



I

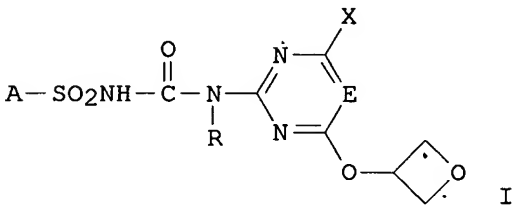
AB Title compds. I (R = Cl, MeO, EtO, PhO, NH2, PhNH; R1 = CH2CN) were prepared in 65-78% yield by reaction of I (R1 = Cl) with tert-Bu cyanoacetate.

L5 ANSWER 10 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:684443 CAPLUS
DN 123:77071
TI Alcoholysis and chemical hydrolysis of chlorimuron-ethyl
AU Sabadie, J.
CS Groupe d'Etudes et de Recherche Appliquees Pluridisciplinaires, UA CNRS 461, Perpignan, 66860, Fr.
SO Weed Research (1995), 35(1), 33-40
CODEN: WEREAT; ISSN: 0043-1737
PB Blackwell
DT Journal
LA English
AB Alcoholysis (MeOH or EtOH) and hydrolysis (pH ≤8) of chlorimuron Et at 30° or 50° involved the breakdown of the urea function. The pyrimidinamine is always obtained in high yield along with the corresponding carbamate (alcoholysis) or phenylsulfonamide (hydrolysis). This compound was easily cyclized to saccharin (pH≥6). In alkaline solution, the carbethoxy substituent of the aromatic ring was preferentially hydrolyzed. The first-order kinetic consts. were characterized. No formation of desmethyl chlorimuron was observed

L5 ANSWER 11 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1994:54558 CAPLUS
DN 120:54558
TI New sulfonylureas useful as herbicides and their preparation
IN Meyer, Willy; Jau, Beat; Kuehlmeyer, Rainer; Pissiotas, Georg; Schurter, Rolf; Foery, Werner
PA Ciba-Geigy A.-G., Switz.
SO Ger. Offen., 26 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 4304864	A1	19930826	DE 1993-4304864	19930217
PRAI CH 1992-521	A	19920220		

OS MARPAT 120:54558
GI



I

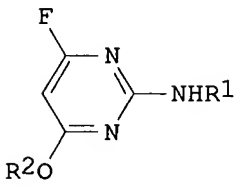
AB Title compds. I [A = various substituted Ph, thienyl, pyridyl, pyrazolyl, imidazopyridyl, sulfonamido, or benzoxathianyl groups; R = H, Me; E = N, CH; X = C1-4 (halo)alkyl or (halo)alkoxy, halo, cyclopropyl, NHMe, NMe2] were prepared as herbicides and plant-growth inhibitors. Thus, etherification of 3-hydroxyoxetane with 2-amino-4-chloro-6-methoxy-1,3-pyrimidine by substitution of chloro, and reaction of the product with 2-(MeO2C)C6H4SO2N:C:O at the amino group, gave title compound I [A = 2-(MeO2C)C6H4, R = H, X = OMe, E = CH]. I are said to show strong pre- and postemergent herbicidal activity against various weeds (no data).

L5 ANSWER 12 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1992:154162 CAPLUS
DN 116:154162
TI Synthesis of 2-aminopyrimidine derivatives
AU Kong, Fanlei; Wang, Lanqing; Hu, Xinhua; Tao, Zhiming; Wang, Xiaoqing; Cao, Weiqun; Dong, Yu
CS Jiangsu Provin. Horm. Inst., Peop. Rep. China
SO Huaxue Shijie (1991), 32(6), 254-7
CODEN: HUAKAB; ISSN: 0367-6358
DT Journal
LA Chinese
AB Production methods for 12 2-aminopyrimidine derivs. by cyclocondensation of guanidine nitrate with acetylacetone, di-Et malonate, or Et acetoacetate were described.

L5 ANSWER 13 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1991:42806 CAPLUS
DN 114:42806
TI Preparation of 2-amino-4-fluoro-6-alkoxypyrimidines
IN Hamprecht, Gerhard
PA BASF A.-G., Germany
SO Ger. Offen., 12 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3900471	A1	19900712	DE 1989-3900471	19890110
	CA 2005596	A1	19900710	CA 1989-2005596	19891214
	CA 2005596	C	19980217		
	US 5011927	A	19910430	US 1989-452106	19891218
	EP 378089	A1	19900718	EP 1990-100075	19900103
	EP 378089	B1	19940629		
	R: BE, CH, DE, FR, GB, IT, LI, NL				
	JP 02225473	A	19900907	JP 1990-720	19900108
PRAI	DE 1989-3900471	A	19890110		

OS CASREACT 114:42806; MARPAT 114:42806
GI



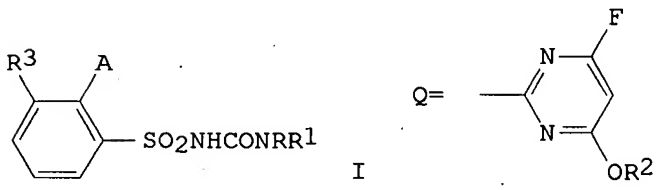
I

AB The title compds. [I; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, (un)substituted Ph, PhCH2; R2 = groups cited for R1 excepting H] were prepared by condensation of 2,4,5-trifluoropyrimidine (II) with R1NH2 at -80° to -15°, separation of isomeric products, and condensation with R2ON in the presence of an (organic) base. Thus, liquid NH3 was added to a solution of II in Et2O at -30° to -20° to give 91% 2-amino-4,6-difluoropyrimidine which was refluxed 5 h in MeON containing NaOMe to give 88% I (R1 = H, R2 = Me).

L5 ANSWER 14 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1990:631401 CAPLUS
DN 113:231401
TI Preparation of N-(2-pyrimidinyl)-N'-(phenylsulfonyl)ureas as herbicides
IN Hamprecht, Gerhard; Westphalen, Karl Otto; Wuerzer, Bruno
PA BASF A.-G., Germany
SO Ger. Offen., 23 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3900472	A1	19900712	DE 1989-3900472	19890110
	CA 2005595	A1	19900710	CA 1989-2005595	19891214
	CA 2005595	C	19990525		
	EP 378092	A1	19900718	EP 1990-100079	19900103
	EP 378092	B1	19940511		
	R: BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
	HU 52763	A2	19900828	HU 1990-75	19900109
	HU 206498	B	19921130		
	JP 02225472	A	19900907	JP 1990-1663	19900110
	JP 2834247	B2	19981209		
PRAI	DE 1989-3900472	A	19890110		

OS CASREACT 113:231401; MARPAT 113:231401
GI



I

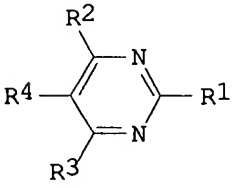
AB The title compds. [I; A = halo, COBR4; B = O, NR5; R = Q; R1 = H, alkyl, alkenyl, alkynyl; R2 = alkyl; R3 = H, halo; R4 = H, (un)substituted alkyl; R5 = H, alkyl; NR4R5 = heterocyclyl] were prepared as herbicides (no data). Thus, Me 6-fluoroanthranilate was diazotized and the product stirred with SO2 and CuCl2 after which Cl was introduced to give 3,2-F(MeO2C)C6H4SO2R6 (II; R6 = Cl) which was treated with NH3 to give II (R6 = NH2). The latter was condensed with QNH2 (R2 = Me) (preparation give) to give I (A = CO2Me, R1 = H, R2 = Me, R3 = F).

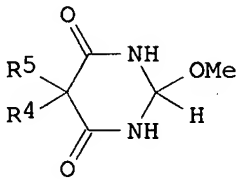
L5 ANSWER 15 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:574117 CAPLUS
DN 111:174117
TI Preparation of 2-amino-4-halo-6-methoxypyrimidine derivatives as materials for drugs and agrochemicals
IN Haga, Takahiro; Tsujii, Yasuhiro; Murai, Shigeo; Yoshizawa, Hiroshi; Tsukada, Sadao
PA Ishihara Sangyo Kaisha, Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

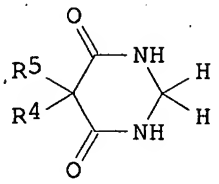
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 01016770	A	19890120	JP 1987-172453	19870710
PRAI	JP 1987-172453		19870710		

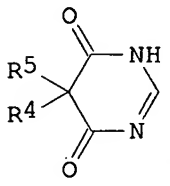
AB The title derivs. and their salts are prepared by treating Me N-cyanocyanoacetimidate (I) with H halides using benzene with 1-3 alkyl and/or halo substituents as the solvent. A solution of 2.46 g I in mesitylene was treated with HCl at -15° over 2 h, then stirred at the same temperature for 30 min to give 2-amino-4-chloro-6-methoxypyrimidine-HCl, which was treated with aqueous NaOH to give 2.25 g 2-amino-4-chloro-6-methoxypyrimidine (II). Then, a solution of 1.84 g II in MeOH was refluxed with KOH for 4.5 h to give 1.76 g 2-amino-4,6-dimethoxypyrimidine.

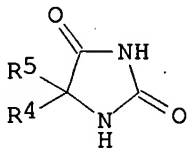
L5 ANSWER 16 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:154253 CAPLUS
DN 110:154253
TI Synthesis and antibacterial effect of derivatives of 5-(3,4,5-trimethoxybenzyl)pyrimidine, -tetrahydropyrimidine, -hexahydropyrimidine and -hydantoin
AU Kujundzic, Nedjeljko; Kovacevic, Krunoslav; Jakovina, Miroslav; Gluncic, Berislav
CS Pliva Res. Inst., Zagreb, Yugoslavia
SO Croatica Chemica Acta (1988), 61(1), 121-35
CODEN: CCACAA; ISSN: 0011-1643
DT Journal
LA English
OS CASREACT 110:154253
GI

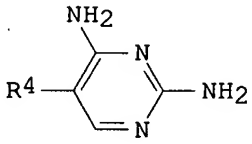

I


II


III

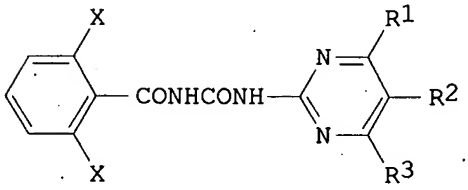

IV


V


VI

AB Pyrimidine derivs. I (R1, R2, R3 = Cl, OMe, NH2, H, OH, R4 = 3,4,5-trimethoxybenzyl), hexahydropyrimidine-4,6-diones II and III (R5 = Me, Et, Pr, CH2CH:CH2, Bu), tetrahydropyrimidine-4,6-diones IV (R5 the same) and hydantoins V (R5 the same) were synthesized. In vitro antibacterial activity of these compds. was tested against some bacteria strains and compared with that of the well known bacteriostatic trimethoprim VI. The activity of compound I (R1 = H, R2 = R3 = OH) was higher than that of trimethoprim against Sarcina lutea ATCC 9341, Klebsiella pneumoniae ATCC 10031 and Pseudomonas aeruginosa NCTC 10490 while the compds. of group IV acted also against Corynebacterium xerosis NCTC 9755, E. coli ATCC 10536 and Shigella flexneri.

L5 ANSWER 17 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:75428 CAPLUS
DN 110:75428
TI N-(2,6-Dihalobenzoyl)-N-pyrimidinylureas
AU Bodenteich, Michael; Chemelli, Elke; Griengl, Herfried
CS Inst. Org. Chem., Tech. Univ. Graz, Graz, A-8010, Austria
SO Monatshefte fuer Chemie (1987), 118(12), 1395-402
CODEN: MOCMB7; ISSN: 0026-9247
DT Journal
LA German
OS CASREACT 110:75428
GI



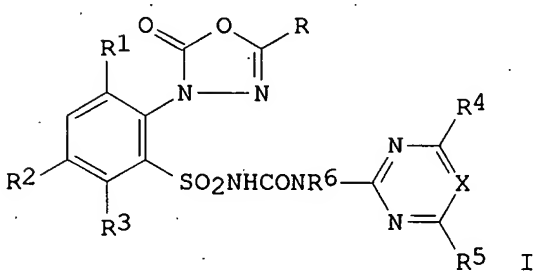
I

AB N-(2,6-Dichlorobenzoyl)- and N-(2,6-difluorobenzoyl)-N'-pyrimidinylureas I (X = F, Cl, R1 = H, Cl, OEt, R2 = H, Cl, OPh, R3 = H, Cl, OPh, Me) have been synthesized by reaction of the corresponding aminopyrimidine derivs. with 2,6-dichlorobenzoyl isocyanate or 2,6-difluorobenzoyl isocyanate. The insecticidal activity of I has been evaluated.

L5 ANSWER 18 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1988:473447 CAPLUS
DN 109:73447
TI Preparation and testing of [(oxadiazolylphenyl)sulfonyl] urea herbicides
IN Borrod, Guy; Guigues, Francois
PA Rhone-Poulenc Agrochimie, Fr.
SO Eur. Pat. Appl., 37 pp.
CODEN: EPXXDW
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 246984	A2	19871125	EP 1987-420117	19870504
	EP 246984	A3	19880302		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	FR 2598416	A1	19871113	FR 1986-6794	19860507
	FR 2605007	A2	19880415	FR 1986-14279	19861010
	JP 62263178	A	19871116	JP 1987-108759	19870501
	ZA 8703213	A	19871230	ZA 1987-3213	19870505
	DK 8702311	A	19871108	DK 1987-2311	19870506
	FI 8702000	A	19871108	FI 1987-2000	19870506
	AU 8772527	A	19871112	AU 1987-72527	19870506
	BR 8702317	A	19880217	BR 1987-2317	19870506
	HU 44138	A2	19880229	HU 1987-2035	19870506
	DD 256255	A5	19880504	DD 1987-302502	19870506
	CN 87103399	A	19871216	CN 1987-103399	19870507
PRAI	FR 1986-6794	A	19860507		
	FR 1986-14279	A	19861010		

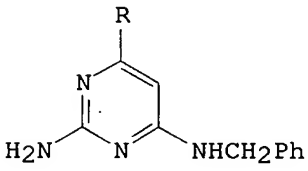
OS CASREACT 109:73447
GI



I

AB The title compds. [I; R = H, (halo)alkyl, alkenyl, alkynyl, alkoxy, alkoxyalkyl; R1-R3 = H, halo, (halo)alkyl, alkoxy(carbonyl); R4, R5 = halo, (halo)alkyl, alkoxy; R6 = H, alkyl; X = CH, N] were prepared as herbicides. 2-(2,3-Dihydro-2-oxo-1,3,4-oxadiazol-3-yl)benzenesulfonamide (preparation given) was treated with COCl2 and BuNCO in xylene containing 1,4-diazobicyclo[2.2.2]octane to give the corresponding benzenesulfonyl isocyanate which was condensed with 2-amino-4,6-dimethylpyrimidine to give I (R-R3 = R6 = H, R4 = R5 = Me, X = CH) (II). In pre- and postemergence tests 125 g II/ha gave 100% control of, e.g., Echinochloa crus-galli and Lolium multiflorum. Application formulations are given.

L5 ANSWER 19 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1986:400162 CAPLUS
DN 105:162
TI Inhibitors of Bacillus subtilis DNA polymerase III. Influence of modifications in the pyrimidine ring of anilino- and (benzylamino)pyrimidines
AU Trantolo, Debra J.; Wright, George E.; Brown, Neal C.
CS Med. Sch., Univ. Massachusetts, Worcester, MA, 01605, USA
SO Journal of Medicinal Chemistry (1986), 29(5), 676-81
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



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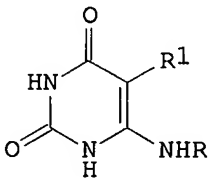
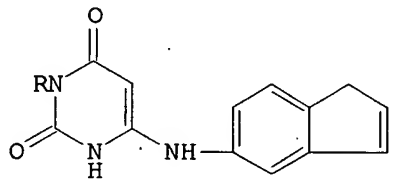


II



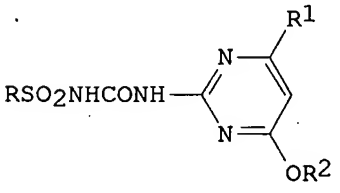
III

AB Of thirty-nine title compds. [I, R = Cl, Me, OPh, NH2, alkoxy, (substituted phenoxy, SMe, SCH2Ph, or SCH2C6H4Cl-4; II, R = H, Me, Et, N; I, Br, etc.; R1 = CH2Ph or C6H4Me-4; III, R = Me, Et, Pr, Bu; 6-(benzylamino)isocytosine; and 6-(5-indanylamino)isocytosine], 33 were prepared (e.g. by reaction of 5-indanylamine [24425-40-9] with the appropriate 3-alkyl-6-chlorouracil or by heating the appropriately prepared 2-amino-4-alkoxy- or 2-amino-4-aryloxy-6-chloropyrimidine with benzylamine [100-46-9]) and tested for inhibitory activity against DNA polymerase III of B. subtilis. Structure-activity relations are discussed. Apparently, the Ph rings of these compds. must exist in conformations in which they are perpendicular to the pyrimidine ring plane; charge-transfer stabilization of such active conformations may compensate for steric barriers from 5-halo groups in the inhibitor-enzyme complex.

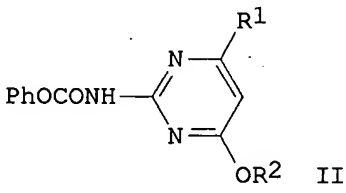
L5 ANSWER 20 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1986:104433 CAPLUS
DN 104:104433
TI Herbicidal halopyrimidines
IN Brown, Hugh Malcolm; Pasteris, Robert James
PA du Pont de Nemours, E. I., and Co., USA
SO Eur. Pat. Appl., 104 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 161905	A2	19851121	EP 1985-303256	19850508
	EP 161905	A3	19860917		
	EP 161905	B1	19900801		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	US 4612035	A	19860916	US 1984-608556	19840509
	US 4659361	A	19870421	US 1985-721602	19850412
	CA 1229086	A1	19871110	CA 1985-480922	19850507
	AU 8542088	A	19851114	AU 1985-42088	19850508
PRAI	US 1984-608556	A	19840509		
	US 1984-619276	A	19840611		
	US 1985-721602	A	19850412		

OS CASREACT 104:104433; MARPAT 104:104433
GI



I.



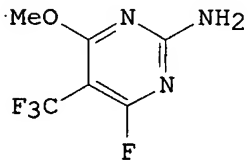
II

AB The sulfonylureidohalopyrimidines I [R = (un)substituted aryl, heterocyclic radical; R1 = iodo, Br; R2 = Me, Et] are herbicides. Thus, I [R = 2,5-(MeO2C)MeC6H3, R1 = iodo, R2 = Me], applied pre-emergently in the greenhouse at 0.05 kg/ha, controlled morningglory (Ipomoea) and purple nutsedge (Cyperus rotundus) with no damage to wheat. I are prepared, e.g., by reacting a sulfonamide RSO2NH2 with a phenyl carbamate II.

L5 ANSWER 21 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1984:611175 CAPLUS
DN 101:211175
TI 2-Amino-4-fluoro-5-trifluoromethyl-6-methoxypyrimidine
PA Nippon Mectron Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 59104366	A	19840616	JP 1982-212525	19821203
PRAI	JP 1982-212525		19821203		

GI



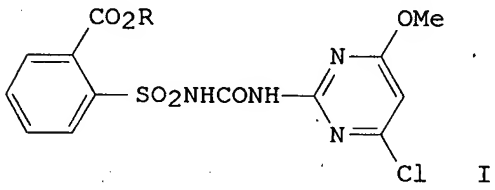
I

AB Title compound (I) was prepared by reaction of (F3C)2C:CFOMe (II) with H2NC(:NH)NH2 (III). Thus, 1 g II in CH2Cl2 and 0.1 g PhCH2N+Me3 Cl- were added to an aqueous mixture of 2 g III carbonate and 0.8 g NaOH and the whole was kept 1 h at room temperature to give 79% I.

L5 ANSWER 22 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1984:455111 CAPLUS
DN 101:55111
TI Pyrimidinylureidosulfonylbenzoates for controlling undesirable plant growth
IN Wolf, Anthony David
PA du Pont de Nemours, E. I., and Co. , USA
SO Braz. Pedido PI, 22 pp.
CODEN: BPXXDX
DT Patent
LA Portuguese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	BR 8303322	A	19840207	BR 1983-3322	19830622
	AU 8316181	A	19840105	AU 1983-16181	19830623
	AU 574645	B2	19880714		
	CA 1229087	A1	19871110	CA 1983-431042	19830623
	SU 1215603	A3	19860228	SU 1983-3609451	19830624
	US 4547215	A	19851015	US 1983-528607	19830906
	US 4645530	A	19870224	US 1985-770258	19850828
PRAI	US 1982-392364	A	19820625		
	US 1983-528607	A2	19830906		

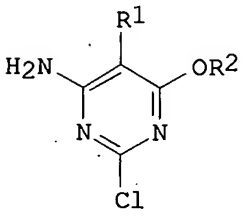
OS MARPAT 101:55111
GI



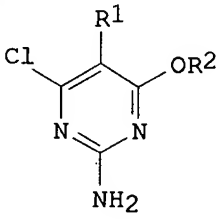
I

AB Title compds. I (R = Et, CHMe2, allyl) were prepared Thus, 2-amino-4,6-dichloropyrimidine was methoxylated and treated with 2-EtO2CC6H4SO2NCO to give I (R = Et). At 0.05 kg/ha post-emergence I (R = Et) gave total control of Xanthium pennsylvanicum.

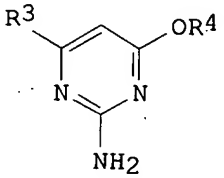
L5 ANSWER 23 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1976:405585 CAPLUS
DN 85:5585
TI A novel synthesis of pyrimidines. II. Cyclization of alkyl N-cyano cyanoacetimidates with hydrogen halides
AU Hirayama, Tadamasa; Kamada, Masahiro; Mimura, Masataka; Tsurumi, Hideaki
CS Res. Inst., Daiichi Seiyaku Co., Ltd., Tokyo, Japan
SO Chemical & Pharmaceutical Bulletin (1976), 24(3), 507-14
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
OS CASREACT 85:5585
GI



II



III



IV

AB Reaction of NCCHR1C(OR2):NH·HCl(R1 = H, Me, Ph; R2 = Me, Et, Pr, CHMe2, Bu) with H2NCN in the presence of a dispersing agent gave NCCHR1C(OR2):NCN(I) in good yields, cyclization of which gave a mixture of the 2-chloropyrimidines II and the 6-chloropyrimidines III, whereas in the presence of a Lewis acid only II were obtained. HBr and HI gave the aminopyrimidinols IV(R3 = Br, R4 = H, Me, Pr; R3 = I, R4 = H, resp.).

L5 ANSWER 24 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1974:520570 CAPLUS
DN 81:120570
TI Novel synthesis of pyrimidines. III. Cyclization of alkyl N-cyanocyanoacetimidates
AU Hirayama, Tadamasa; Kamada, Masahiro; Mimura, Masataka; Tsurumi, Hideaki
CS Res. Inst., Daiichi Seiyaku Co., Ltd., Tokyo, Japan
SO Heterocycles (1974), 2(4), 461-6
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB The treatment of cyanoacetimidates, NCCHRC(OR1):NH.HCl, with H2NCN gave the N,2-dicyanoacetimidates, NCCHRC(OR1):NCN (I), which, treated with HX in a nonpolar solvent such as ether or benzene, gave halo pyrimidines II (R = H, Me, Ph; R1 = Me, Et, Pr, Me2CH; R2 = Cl, Br). Treatment of II (R = H, R1 = Me) with HBr in a polar solvent such as HOAc unexpectedly gave 2-amino-6-bromo-4-methoxypyrimidine and 2-amino-6-bromo-4-hydroxypyrimidine.

L5 ANSWER 25 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1972:34191 CAPLUS
DN 76:34191
TI Pyrimidine derivatives. XVII. 2-Amino-4,6-dihydroxy-5-(p-alkoxybenzyl)pyrimidines and some of their reactions
AU Aroyan, A. A.; Kaldrikyan, M. A.; Grigoryan, L. A.
CS Inst. Tonkoi Org. Khim. im. Mndzhoyana, Erevan, USSR
SO Armyanskii Khimicheskii Zhurnal (1971), 24(8), 721-6
CODEN: AYKZAN; ISSN: 0515-9628
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB The title compds. I (R1=R2=OH) (II) were prepared in 86-91% yield by treating H2NC(:NH)NH2.HCl with p-alkoxybenzylmalonic esters in presence of 3 equivalent of NaOEt. Prolonged boiling of II with POCl3 gave I (R1=R2=Cl), which reacted with NaOEt, NH2NH2.H2O or ethylenimine to produce I (R1=Cl, R2=OEt), I (R1=Cl, R2=NHNH2) or I (R1=Cl, R2=1-aziridinyl), resp.

L5 ANSWER 26 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1968:95774 CAPLUS
DN 68:95774
TI 5-Cyanopyrimidine derivatives through the cyclization of 1-cyanamino-2,2-dicyanoethylenes
AU Allenstein, Eckhard; Fuchs, Rainer
CS Univ. Stuttgart, Stuttgart, Fed. Rep. Ger.
SO Chemische Berichte (1968), 101(4), 1244-9
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
OS CASREACT 68:95774
AB 1-Ethoxy, 1-(methylamino), and 1-(dimethylamino) derivs. of Na 1-cyanamino-2,2-dicyanoethylenides or the free acids were cyclized by treatment with HCl, giving the 6-ethoxy, 6-(methylamino), and 6-(dimethylamino) derivs. of 4-chloro-2-amino-5-cyanopyrimidine. Similarly, Na 1-amino-1-cyanamino-2,2-dicyanoethylenide gave 4,6-diamino-2-chloro-5-cyanopyrimidine. Further derivs. were prepared by substituting EtO and NH2 groups for the Cl on the pyrimidine obtained.

L5 ANSWER 27 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1966:490645 CAPLUS
DN 65:90645
OREF 65:16966b-h,16967a-e
TI Pyrimidines series. XVIII. Synthesis and reactions of 4-chloro-5-nitropyrimidines
AU Buehler, Eberhard; Pfleiderer, Wolfgang
CS Tech. Hochsch., Stuttgart, Germany
SO Chemische Berichte (1966), 99(9), 2997-3007
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
GI For diagram(s), see printed CA Issue.
AB cf. preceding abstract The synthesis of new 4-chloro-5-nitropyrimidines is described; their reactivity towards various nucleophilic reagents was investigated. 4-Chloro-1,3-dimethyluracil (I) (42.5 g.) in 125 cc. concentrated H2SO4 treated <15° with stirring dropwise with 42 cc. fuming HNO3 (d. 1.5) and stirred into 500-600 g. ice yielded 49.5 g. (crude) pale yellow 5-NO2 derivative of I, m. 80-3° (sublimed in vacuo at 70-5°). 2-Amino-4-chloro-6-methoxypyrimidine (II) (3 g.) in 6 cc. concentrated H2SO4 treated dropwise at room temperature with 3 cc. fuming HNO3, heated 15 min. at 65-70°, cooled to 0°, and stirred into 50 g. crushed ice gave 1 g. pale yellow 5-NO2 derivative (III) of II, m. 177-9° (sublimed at 90°/0.01 mm.). 4-Chloro-6-methoxy-2-nitraminopyrimidine (IV) (0.5 g.) in 1 cc. H2SO4 heated 15 min. at 70° and poured onto ice gave pale yellow III, m. 177-9° (H2O). 4-Chloro-2-dimethylamino-6-methoxypyrimidine (V) (10 g.) in 20 cc. concentrated H2SO4 treated dropwise at 0-5° with 10 cc. fuming HNO3 gave 6.6 g. light yellow 5-NO2 derivative (VI) of V, m. 114-16° (EtOH). II (5 g.) in 10 cc. concentrated H2SO4 treated at 0-5° with 5 cc. fuming HNO3 and kept 1 hr. at room temperature yielded 2.4 g. IV, m. 120-2° (ligroine). IV (1 g.) in 60 cc. EtOH hydrogenated at room temperature over Raney Ni gave 0.55 g. II, m. 165°. 2,6-Diamino-4-chloropyrimidine (VII) (4 g.) in 8 cc. concentrated H2SO4 treated slowly with stirring and cooling with 4 cc. fuming HNO3 yielded 2.5 g. pale yellow 2-O2NNH analog of VII, m. 227°. Guanidine carbonate (VIII) (0.88 g.), 0.22 g. Na, and 30 cc. EtOH refluxed 10 min., treated with 1 g. 2-amino-4-chloro-1-methyl-5-nitro-6-oxodihydropyrimidine (IX), and refuxed 2 hrs. gave 0.25 g. yellow 4-H2NC(:NH)NH analog of IX, m. 229-31° (decomposition) (H2O). IX (2 g.) and 0.75 g. urea in 40 cc. EtOH refluxed 0.5 hr. and kept overnight yielded 1.75 g. pale yellow 4-H2NC(:NH)O analog of IX, m. 187-9° (decomposition) (EtOH). VIII (5.25 g.), 1.35 g. Na, and 120 cc. EtOH refluxed 10 min., treated with 6 g. 4-chloro-2-dimethylamino-5-nitropyrimidine, refluxed 1 hr., and kept overnight gave 3 g. light yellow needles, m. 191-3° (decomposition). N-(2-Amino-1-methyl-4-nitro-6-oxo-4-dihydropyrimidinyl)pyridinium chloride (1.4 g.) in 50 cc. absolute EtOH refluxed 1.5 hrs. with 1.3 cc. PhNH2 yielded 0.8 g. 2-amino-4-anilino-1-methyl-5-nitro-6-oxodihydropyrimidine (X), m. 292-4° (decomposition) (EtOH). IX (1 g.) and 1.3 cc. PhNH2 in 45 cc. EtOH refluxed 0.5 hr. yielded 0.95 g. X. 2-Amino-4-chloro-5-nitro-6-oxodihydropyrimidine (XI) (1 g.) and 4 g. 2-aminopyridine (XII) in 100 cc. absolute EtOH refluxed 75 min. gave 0.45 g. 4-(2-pyridylamino) analog (XIII) of XI, m. 305-7° (decomposition). XIII (1 g.) in 50 cc. MeOH hydrogenated at room temperature over Raney Ni, treated with 2 cc. AcCO2Et, filtered, and refluxed 1.5 hrs. yielded 0.2 g. pale yellow XIV, m. from 305° (decomposition). 4-Chloro-2-dimethylamino-5-nitropyrimidine (XV) (2 g.) and 4 g. XII fused about 10 min. at 70° gave 1.3 g. 4-(2-pyridylamino) analog (XVI) of XV, m. 210-12°. XV (2 g.) and 4 g. 3-aminopyridine gave similarly

1.8 g. pale yellow 4-(3-pyridylamino) analog of XV, m. 219-21° (EtOH). 2-Amino-4-chloro-6-methoxy-5-nitropyrimidine (0.5 g.) and 2 g. XII fused at 100° gave 0.25 g. pale yellow 4-(2-pyridylamino) analog of II, m. 213-15° (EtOH). XVI (0.5 g.) in 30 cc. MeOH hydrogenated over Raney Ni, treated with 0.5 cc. AcCO2Et, filtered, and refluxed 0.5 hr. yielded 0.15 g. pale yellow XVII, m. 203-4° (decomposition) (ligroine). 2,4,5-Triamino-1-methyl-6-oxodihydropyrimidine dihydrochloride (4.6 g.), 0.92 g. Na, and 100 cc. EtOH refluxed 15 min., cooled to room temperature, treated with 2 g. IX, and refluxed 40 min. gave 2.2 g. light yellow XVIII, m. >350° (decomposition) (2N HCl). XV (1 g.) and 1.5 g. 4,6-diamino-2-dimethylaminopyrimidine (XIX) in 50 cc. BuOH refluxed 4 hrs., cooled overnight, and filtered, and the residue boiled with 750 cc. xylene left XIX. HCl; the filtrate deposited overnight 0.33 g. orange XX, m. 241-3° (EtOH). XI (0.5 g.) in 6 cc. dry HCONMe2 heated 5 min. at 80° with 1 cc. absolute C5H5N gave 0.5 g. XXI (R = H) (XXII), m. 210° (decomposition). XXII (0.55 g.) in 8 cc. H2O adjusted with solid NaHCO3 to pH 8-9 and kept several hrs. at room temperature yielded 0.15 g.

yellow N-(2-amino-5-nitro-6-oxo-4-pyrimidinyl)pyridinium betaine, m. >200° (decomposition) (H2O). IX (0.5 g.) in 7 cc. dry C5H5N heated briefly to boiling yielded 0.7 g. light yellow XXI (R = Me) (XXIII), m. 200-2° (decomposition). XV (0.5 g.) in 5 cc. dry C5H5N gave similarly 0.6 g. XXIV, m. 163-4°. 4-Chloro-5-nitrouracil (XXV) (1 g.) in 5 cc. dry HCONMe2 and 2 cc. dry C5H5N heated to 80° gave 0.8 g. light yellow XXVI (R = R' = R'' = H) (XXVII), m. 251° (decomposition) (H2O). XXV (1 g.), 1. cc. 3-picoline, and 5 cc. HCONMe2 gave similarly 0.75 g. light yellow XXVI (R = R'' = H, R' = Me) (XXVIII), m. >260° (decomposition) (H2O). XXV (1 g.) and 1.5 cc. dry 4-picoline in 5 cc. HCONMe2 yielded 0.75 g. yellow XXVI (R = R' = H, R'' = Me) (XXIX), m. from 240° (decomposition) (H2O). 1-Me derivative (0.5 g.) of XXV, 1 cc. dry C5H5N, and 4 cc. dry HCONMe2 gave similarly 0.45 g. light yellow XXVI (R = Me, R' = R'' = H) (XXIXa), m. 260° (decomposition) (H2O). XXII (1 g.) in 15 cc. H2O refluxed 10 min. gave 0.5 g. 2-amino-4-hydroxy-5-nitro-6-oxodihydropyrimidine (XXX), m. above 350°. XXIII (0.85 g.) in 10 cc. H2O refluxed 5 min. yielded 0.4 g. 1-Me derivative (XXXI) of XXX, m. 300-2° (decomposition) (H2O). IX (3 g.) in 30 cc. N NaOH refluxed 1 hr. and acidified with 2N HCl gave 0.5 g. XXXI, m. 297° (decomposition) (very dilute HCl). XI (0.4 g.) in 100 cc. MeOH and 5 cc. dry C5H5N refluxed 0.45 min. gave 0.3 g. 2-amino-4-methoxy-5-nitro-6-oxodihydropyrimidine (XXXII), m. from 274° (decomposition) (H2O). IX (1.2 g.) in 25 cc. MeOH refluxed 50 min. with 5 cc. dry C5H5N gave 0.6 g. lemon-yellow 1-Me derivative (XXXIII) of XXXII, m. 214-16° (MeOH). XXIV (1.5 g.) in 20 cc. absolute EtOH refluxed briefly with 1.1 g. XII yielded 0.3 g. orange XXXIV, m. 154-6° (decomposition) (CHCl3). XV (3 g.) and 0.48 g. Na in 20 cc. EtOH refluxed 45 min. gave 1.9 g. pale yellow 4-EtO analog (XXXV) of XXXIV, m. 104-6° (sublimed at 80° in vacuo). XXIV (2.2 g.) in 5 cc. absolute EtOH refluxed 1.5 hrs. gave 0.5 g. XXXV. The pK values in H2O at 20° (given) were determined for the following compds.: XXVII -0.80 ± 0.07, XXVIII -0.12 ± 0.05, XXIX 0.14 ± 0.01, XXIXa -0.39 ± 0.1, XXII, 3.16 ± 0.18, XXXI 5.55 ± 0.07, XXXII 7.41 ± 0.07, XXXIII 1.25 ± 0.04, XIV 8.15 ± 0.09, XVII 2.04 ± 0.02.

L5 ANSWER 28 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1966:104289 CAPLUS
DN 64:104289
OREF 64:19637d-h,19638a-b
TI Pyrimidine derivative tranquilizers
IN Tedeschi, David H.
PA Smith Kline & French Laboratories
SO 13 pp.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	BE 657135		19650615	BE	19641215
	GB 1034608			GB	
PRAI	US		19631226		

OS MARPAT 64:104289
GI For diagram(s), see printed CA Issue.
AB Pyrimidine derivs. with general formula (I) are prepared A mixture of 12 g. NaOMe, 125 cc. MeOH, and 27.2 g. 1,1-dimethylguanidine sulfate is refluxed for 0.5 hr., cooled, 31.6 g. ethyl acetoacetate (II) added, and the mixture refluxed for 23 hrs. with stirring. The cooled mixture is diluted with 100 cc. water and acidified with AcOH to give 2-(N,N-dimethylamino)-4-hydroxy-6-methylpyrimidine (III). A solution of 4.6 g. III in 20 cc. POCl3 is refluxed for 4 hrs., cooled, poured onto 100 g. ice, and neutralized. The solution is extracted with ether, the extract dried and evaporated to dryness, and the residue sublimed to give 2-(N,N-dimethylamino)-4-chloro-6-methylpyrimidine, m. 35-6°; hexamate m. 212° (decomposition). The reaction of 2-ethylthio-4-hydroxy-6-methylpyrimidine (IV) with dimethylamine under pressure in a solvent gives III. A mixture of 6 g. guanidine carbonate, 10.2 g. trifluoroethylacetone, and 15 cc. trifluoroacetylacetone is refluxed 1.75 hrs. to give 2-amino-4-methyl-6-trifluoromethylpyrimidine, m. 120-4°. 2-Amino-4,6-dichloropyrimidine (5.8 g.) is added slowly to a cooled solution of 3.85 g. NaOMe in 25 cc. MeOH. The mixture is stirred 24 hrs. at room temperature The precipitate is separated, washed with MeOH and water, and sublimed in vacuo to give 2-amino-4-chloro-6-methoxypyrimidine, m. 172-4°. A solution of 500 g. EtI in 2 l. ether is added slowly to a mixture of 93.5 g. Mg in 250 cc. ether, and the mixture refluxed 45 min. A solution of 140 g. ethyl cyanoacetate in 375 cc. ether is added slowly, and refluxing continued for an addnl. 1 hr. The cooled solution is poured into ice, acidified with concentrated H2SO4, and decanted. The ethereal layer is dried and evaporated to give ethyl propionylacetate (V), b38-40 98-108°. A mixture of 43.3 g. V, 55.4 g. guanidine carbonate, and 330 cc. anhydrous EtOH is refluxed for 18 hrs., 60 cc. water added, and the mixture refluxed 2 hrs. to give 2-amino-4-hydroxy-6-ethylpyrimidine (VI), m. 249-51°. The reaction of VI with POCl3 gives 2-amino-4-chloro-6-ethylpyrimidine, m. 121-3°. A mixture of 200 cc. HCONMe2, 5.4 g. NaOMe, 27.2 g. 1,1-dimethylguanidine sulfate, and 41.7 g. diethyl malonate is refluxed 5 hrs. to give 2-(N,N-dimethylamino)-4,6-dihydroxy-pyrimidine (VII), m. 356°. The reaction of VII with POCl3 gives 2-(N,N-dimethylamino)-4,6-dichloropyrimidine, m. 55-6°. A mixture of 100 g. methylguanidine sulfate, 500 cc. HCONMe2, and 44.2 g. NaOMe is refluxed, cooled, 53 g. II added, and the mixture refluxed for 5 hrs. to give 2-methylamino-4-hydroxy-6-methylpyrimidine (VIII). The reaction of VIII with POCl3 gives 2-methylamino-4-chloro-6-methylpyrimidine, m. 135-5.5°. The reaction of IV with methylamine under pressure in a solvent gives VIII. A solution of 10 g. IV, and 20 cc. aqueous ethylamine

(containing 8.9 g. Et2NH) in 25 cc. Cellosolve is heated at 170-80° under pressure for 8 hrs. The solution is evaporated to dryness, and the residue dissolved in ether and crystallized to give 2-ethylamino-4-hydroxy-6-methylpyrimidine (IX), m. 170-4°. The reaction of IX with POCl3 gives 2-ethylamino-4-chloro-6-methylpyrimidine, m. 92.5-4.5°. Similarly prepared were 2-propylamino-4-chloro-6-methylpyrimidine, m. 49-50.5°; 2-amino-4-bromo-6-methylpyrimidine (EtOH), m. 152.5-4°; 2-cyclopropylamino-4-hydroxy-6-methylpyrimidine, m. 220-3°; 2-cyclopropylamino-4-chloro-6-methylpyrimidine, b0.14 82° (hydrochloride m. 174-6°); 2-isopropylamino-4-hydroxy-6-methylpyrimidine; 2-iso-propylamino-4-chloro-6-methylpyrimidine, b0.2 68-72° (hydrochloride, m. 100-2°); 2-(N-ethyl-N-methylamino)4-hydroxy-6-methylpyrimidine, m. 152-5°; 2-(N-ethyl-N-methylamino)-4-chloro-6-methylpyrimidine, b0.3 58-9°. Lactose and Mg stearate are used in the pharmacological prepns.

L5 ANSWER 29 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1963:482241 CAPLUS
DN 59:82241
OREF 59:15274b-c
TI Pyrimidines. I. The synthesis of 6-fluorocytosine and related compounds
AU Wempen, Iris; Fox, Jack J.
CS Cornell Univ. Med. Coll., New York, NY
SO Journal of Medicinal Chemistry (1963), 6(6), 688-93
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA Unavailable
OS CASREACT 59:82241
GI For diagram(s), see printed CA Issue.
AB Syntheses of 6-fluorocytosine (I) and 6-fluoroisocytosine from 2,4,6-trifluoropyrimidine and the preparation of a number of mono- and difluoropyrimidine intermediates are described. 5-Chlorocytosine and 5-chloroisocytosine were obtained from cytosine or isocytosine by use of N-chlorosuccinimide in AcOH. The relative effects of a 5- and 6-halo atom on the ultraviolet absorption spectra and apparent pK8 values of cytosine and isocytosine are presented.

L5 ANSWER 30 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1963:27305 CAPLUS
DN 58:27305
OREF 58:4560c-e
TI Sulfanilamide derivatives. I. Reaction of 6-chloro-2,4-dimethoxypyrimidine with sodium amide in liquid ammonia
AU Okuda, Noriyuki; Kuniyoshi, Ieji
CS Daiichi Pharm. Co., Tokyo
SO Yakugaku Zasshi (1962), 82, 1031-4
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Unavailable
AB A mixture of 2.5 g. 6-chloro-2,4-dimethoxypyrimidine (I) and 40 cc. liquid NH3 is kept 22 hrs. at 20-4° in an autoclave to give 0.1 g. 2-amino-4-methoxy-6-chloropyrimidine (II), needles, m. 169-70° (C6H6). A mixture of 12.4 g. I, 8.4 g. NaNH2, and 30 cc. liquid NH3 in an autoclave is kept 12 hrs. at 10° with occasional shaking to give 4.9 g. 2-amino-4,6-dimethoxypyrimidine (III), m. 94.5-96° (H2O), besides a small amount of such by-products as 6-amino-2,4-dimethoxypyrimidine, 4-methoxy-2,6-diaminopyrimidine (IV) (picrate m. 242°), and 2-methoxy-4,6-diaminopyrimidine (picrate m. 212°). Reaction of 1.75 g. I with 1.2 g. NaOMe in 30 cc. liquid NH3 at room temperature 12 hrs. gives 1.7 g. 2,4,6-trimethoxypyrimidine (V), m. 53°. Reaction of 1.7 g. V with 0.55 g. NaNH2 in 20 cc. liquid NH3 gives 1.2 g. III. Similarly is obtained IV by treating II with NaNH2 in liquid NH3. Considering these results, the mechanism of reactions from I to III is suggested; the MeO group which is attacked by NaNH2 at either 2- or 4-position of I reacted with the unreacted I to yield V, then occurred the secondary reaction between V and excess NaNH2 to give III.

L5 ANSWER 31 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1962:25089 CAPLUS
DN 56:25089
OREF 56:4752b-i,4753a-h
TI Pteridines. XV. Synthesis of 2-amino-4-alkoxy-7-oxodihydropteridines
AU Pficiderer, Wolfgang; Lohrmann, Rolf
CS Tech. Hochschule, Stuttgart, Germany
SO Chemische Berichte (1961), 94, 2708-21
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA Unavailable
OS CASREACT 56:25089
AB cf. CA 55, 551g, 10462f.-The synthesis of 2-amino-4-alkoxy-7-oxodihydropteridine derivs. was described and their structure discussed on the basis of the ultraviolet absorption spectra. 4,6-Dichloro-2-aminopyrimidine (I) (50 g.) in 220 g. 10% MeNH2 in PrOH kept at room temperature overnight, warmed slowly, heated 2 hrs. on the water bath, evaporated, the residue dissolved in about 350 cc. hot H2O, the solution treated with C, filtered, and cooled slowly gave 40 g. 6-chloro-2-amino-4-methylaminopyrimidine (II), m. 162-4° (H2O). I (60 g.), 120 cc. 33% aqueous MeNH2, and 300 cc. 2:1 MeOH-H2O stirred 4 hrs. at 60-80°, filtered hot, and cooled gave 36 g. crude II. I (50 g.) in 200 cc. EtOH refluxed 3 hrs. with 45 g. H2NCH2CH2OH and worked up in the usual manner gave 47 g. 4-(HOCH2CH2NH) analog (III) of II, m. 149-51° (H2O). I (40 g.) refluxed 2.5 hrs. with 6.2 g. Na in 300 cc. iso-PrOH, concd, in vacuo to 80°, acidified with dilute AcOH, and cooled gave 45 g. 4-chloro-2-amino-6-isopropoxypyrimidine (IV), needles, m. 85-6° (aqueous MeOH). II (70 g.) heated 8 hrs. at 150-60° in an autoclave with 11.2 g. Ha in 700 cc. isoPrOH, filtered hot, concd, in vacuo, and diluted with a little xylene gave 71 g. 4-MeNH analog (V) of IV, m. 105-7° (CCl4-petr. ether). II (60 g.) and 9.6 g. Na in 600 cc. MeOH gave similarly 57 g. 6-MeO analog (VI) of V, m. 135-7° (xylene). V (53 g.) in 500 cc. 10% AcOH treated dropwise with stirring at 40° with 22 g. NaNO2 in about 30 cc. H2O, the mixture neutralized with solid NaHCO2, cooled, and filtered gave 41 g. 5-NO derivative (VII) of V, violet, m. 180-1° (decomposition) (xylene). VI (55 g.) in 150 cc. 15% AcOH treated dropwise with stirring at 70-80° with 28 g. NaNO2 gave similarly 46 g. 5-NO derivative (VIII) of VI, violet needles, m. 210-11° (H2O). III (10 g.) heated 7 hrs. in an autoclave at 140-50° with 1.4 g. Na in 200 cc. iso-PrOH, neutralized with AcOH, filtered, evaporated in vacuo, the residue treated with aqueous NANO2 at 50-60°, and the product isolated with CHCl3 yielded the violet 5-NO derivative (IX) of III, m. 150-8° (CHCl3-CCl4). VII (15 g.) in 200 cc. MeOH hydrogenated over Raney Ni yielded 13.8 g. light yellow 5-NH2 derivative (X) of V, m. 96-8° (ligroine). VIII (15 g.) gave similarly 13.1 g. 5-NH2 derivative of VI, needles, m. 171-3° (xylene). 2,4,5-Triamino-6-isopropoxypyrimidine (XI) (2 g.) in 80 cc. MeOH refluxed 4 hrs. with 1.8 g. EtO(HO)CHCO2Et (XII), concentrated to half-volume, and refrigerated 12 hrs. yielded 1.4 g. 2-amino-4-isopropoxy-7-oxodihydropteridine (XIII), m. above 360° (PhCH2OH). 5-Nitroso-2,4-diamino-6-isopropoxypyrimidine (6 g.) in 200 cc. MeOH hydrogenated over Raney Ni, filtered, refluxed 2 hrs. with 4.8 g. BzCO2Et, and refrigerated overnight gave 6.7 g. 6-Me derivative (XIV) of XIII, m. above 360° (PhCH2OH). XI (2 g.) in 80 cc. 50% MeOH refluxed 2.5 hrs. with 2.1 g. CO(CO2Et)2 (XV) gave 1.0 g. 6CO2Et analog (XVI) of XIV, m. above 320° (decomposition). XVI (1 g.) in 150 cc. 0.6M NaHCO3 heated 4 hrs. on the water bath, filtered, acidified hot with 50% AcOH, and kept overnight yielded 0.64 g. 6-CO2H analog (XVII) of XIV, m. above 360° (aqueous HCONMe2). VIII (2.5 g.) in 150 cc. MeOH hydrogenated over Raney Ni, filtered, refluxed 2 hrs. with 2.3 g. XII, concentrated, and kept

overnight gave 2.1 g. 8-methyl-2-amino-4-methoxy-7-oxodihydropteridine (XVIII), light yellow needles, m. 262-6° (decomposition) (aqueous EtOH). VIII (2.5 g.) in 150 cc. MeOH hydrogenated over Raney Ni, filtered, refluxed 2 hrs. with 2 g. BzCO2Et, and concentrated gave 2.2 g. 6-Me derivative (XIX) of XVIII, m. 258-62° (decomposition) (aqueous EtOH). VIII (5 g.) in 200 cc. MeOH hydrogenated over Raney Ni, filtered, refluxed 5 hrs. with 5 g. XV, and concd, gave 6.5 g. 6-CO2Et analog (XX) of XIX, yellow, m. 254-7° (decomposition) (CHCl3-petr. ether). XX (3.4 g.) in 300 cc. N NaHCO2 heated 2 hrs. on the water bath, filtered hot, acidified with AcOH, concentrated, and cooled yielded 2 g. 6-CO2H analog (XXI) of XIX, yellow, m. 252-4° (decomposition) (aqueous HCONMe2). VII (2.5 g.) in 150 cc. MeOH hydrogenated over Raney Ni, filtered, refluxed 1.5 hrs. with 1.9 g. XII, concentrated in vacuo to 15 cc., diluted with 40 cc. xylene, treated with C, concentrated to about 15 cc., and cooled overnight gave 0.35 g. light yellow 8-Me derivative (XXII) of XVI, m. 232-4° (ligroine). X (1 g.) and 0.7 g. BzCO2Et in 50 cc. MeOH refluxed 0.5 hr., poured into 150 cc. hot H2O, and cooled gave 0.9 g. 6-Me derivative (XXIII) of XXII, cream needles, m. 243-5° (aqueous EtOH). VII (5 g.) in MeOH hydrogenated over Raney Ni, filtered, treated with 5 g. XV, the mixture concentrated to half volume, diluted with 25 cc. H2O, refluxed 1 hr., and cooled yielded 4.8 g. 6-CO2Et derivative (XXIV) of XXII, m. 192-4° (ligroine). XXIV (4 g.) in 200 cc. N NaHCO3 heated 2 hrs. on the water bath, cooled, acidified with 40 cc. 50% AcOH, and cooled to 0° gave 3.5 g. crude product, which extracted with CHCl3 and recrystd. from aqueous HCONMe2 gave the 6CO2H derivative (XXV) of XXII, light yellow needles, m. 246-7° (decomposition). IX (1.8 g.) in 150 cc. MeOH hydrogenated over Raney Ni, filtered, refluxed 1 hr. with 2.5 cc. BzCO2Et, concentrated to 20 cc., and cooled yielded 1.25 g. 8-(2-hydroxyethyl)-2-amino-4-isopropoxy-6-methyl- 7-oxodihydropteridine (XXVI), m. 229-31° (aqueous EtOH). XI (2 g.) in 25 cc. (CO2Et)2 heated 10-15 min. at 160-80° gave 2.3 g. 2-amino-4-isopropoxy-6, 7-dioxotetrahydropteridine (XXVII), pale yellow, m. above 360° (4:1 glycol-H2O). X (2.5 g.) in 25 cc. (CO2Et)2 heated slowly to 180°, kept 15 min. at 180°, cooled, and filtered yielded 2.7 g. (crude) 8-Me derivative (XXVIII) of XXVII, m. 244-7° (decomposition) (ligroine). 5-Nitroso-2,4-diamino-6-isopropoxypyrimidine (XXIX) in 40 cc. NCCH2CO2Me heated to near boiling, cooled after 10 min., and filtered gave 1.4 g. 6-CN derivative (XXX) of XIII, yellowish, decomposed above 250° (HCONMe2). XXIX (2 g.) and 4 g. CH2(CN)2 in 20 cc. EtOCH2CH2OH heated slowly to 120-30°, cooled slightly after 15 min., poured into hot H2O, kept several hrs., and filtered yielded 1.1 g. 2,7-diamino-4-isopropoxy-6-cyanopteridine (XXXI), decomposed above 220° (aqueous EtOH). The ultraviolet absorption spectra of the neutral mols. and cations of XVI, XVII, XXIV, XXV, and XXX were recorded. The Rf in 2:1 BuOH-5N AcOH, PrOH-1% NH3, 4% aqueous Na citrate, and 3% aqueous NH4Cl (given in this order) and the pK values in H2O at 20° at the pH indicated in parentheses were determined for the following compds.: XIII, 0.67, 0.55, 0.39, 0.45, 0.74 ± 0.16 (-1.9), 7.60 ± 0.2 (5.0); XIV, 0.68, 0.56, 0.38, 0.42, 1.14 ± 0.13 (-0.89), 7.8 ± 0.2 (5.0); XXII, 0.84, 0.82, 0.52, 0.60, 0.17 ± 0.15 (-1.9); XXIII, 0.86, 0.85, 0.52, 0.56, 0.40 ± 0.18 (-1.9); XVIII, 0.61, 0.66, 0.36, 0.40, 0.21 ± 0.08 (-1.9); XIX, 0.69, 0.72, 0.42, 0.43, 0.55 ± 0.2 (-1.9); XXVI, 0.83, 0.87, 0.63, 0.63, 0.74 ± 0.1 (-1.9): XVII, 0.42, 0.27, 0.62, 0.59, 0.35 ± 0.13 (-1.9), 3.71 ± 0.11 (2.0), 8.32 ± 0.06 (6.0); XVI, 0.75, 0.62, 0.49, 0.53, 0.35 ± 0.12 (-1.9), 7.8 ± 0.2 (3.0); XXV, 0.65, 0.50, 0.71, 0.75, -0.76 ± 0.12 (-2.7), 3.53 ± 0.08 (1.0); XXIV, 0.83, 0.85, 0.62, 0.64, -0.46 ± 0.08 (-2.7); XXI, 0.32, 0.28, 0.55, 0.63, -0.4 ± 0.1 (-2.7), 3.86 ± 0.13 (1.0); XX, 0.69, 0.74, 0.53, 0.54, -0.60 ± 0.1 (-2.7); XXX, 0.72, 0.56, 0.28, 0.38, -0.17 ± 0.08 (-1.9), 5.95 ± 0.13 (4.0);

XXXI, 0.69, 0.71, 0.26, 0.29, 41.0 ± 0.13 (2.0); XXVII, 0.50, 0.32, 0.40, 0.45, 0.82 ± 0.07 (-1.9), 8.46 ± 0.14 (4.0), 12.2 ± 0.2 (10.0); XXVIII, 0.73, 0.62, 0.52, 0.60, 0.53 ± 0.11 (-1.9), 8.53 ± 0.09 (6.0); 1,3,6-trimethyl-7-hydroxy-2,4-dioxotetrahydropteridine, 0.70, 0.50, 0.50, 0.60, -. The various dihydropteridine derivs. showed at 254 and 365 mμ blue fluorescence, while XXVII and XXVIII fluoresced gray except in 4% aqueous Na citrate where the fluorescence was also blue.

L5 ANSWER 32 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1954:77653 CAPLUS
DN 48:77653
OREF 48:13693e-g
TI The catalytic reduction of 2-amino-4,6-dichloropyrimidine in the presence of palladium
AU Kitani, Kazuo; Sodeoka, Hiroshi
CS Mitsui Chem. Ind. Co., Omuta
SO Nippon Kagaku Kaishi (1921-47) (1953), Pure Chem. Sect. 74, 624-6
CODEN: NIKWAB; ISSN: 0369-4208
DT Journal
LA Unavailable
AB H with 3.0 g. 2-amino-4,6-dichloropyrimidine (I) in the presence of 6.3 g. Pd-CaCO3 (containing 12 mg. Pd/g.) and 3.0 g. KOH in 180 cc. MeOH at room temperature gave in less than 1 hr. 1.2 g. 2-amino-pyrimidine (II), m. 123-5° (127-8° after recrystn. from C6H6). In water instead of MeOH, the reaction was slower, but pure II was obtained in a higher yield (1.45 g.), m. 127-8°. In the presence of 1.25 g. Pd-CaCO3 in MeOH-KOH, the products were II, 2-amino-4-methoxy-6-chloropyrimidine (III), m. 170-1° (from aqueous alc.), and 2-amino-4-methoxypyrimidine (IV), m. 120-1° (from H2O). This was due to the concurrent substitution of Cl by MeO. In fact, I and MeOH-KOH gave 87.5% III in 6 hrs. at room temperature; similarly, in the 4-EtO analog, m. 89-90°, was obtained in EtOH-KOH. III was dechlorinated to IV with H and PdCaCO3. In the absence of KOH, other conditions being the same as in the 1st experiment, I was reduced to 2-aminohexahydropyrimidine, which was characterized as the picrate C4H11N3.C6H3N3O7, m. 179-80°, and carbonate, (C4H11N3)2.H2CO3, m. 237° (decomposition).

L5 ANSWER 33 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1946:17714 CAPLUS
DN 40:17714
OREF 40:3413e-i,3414a-e
TI p-Aminobenzenesulfonamide derivatives of pyrimidine as antibacterial agents
AU Rose, F. L.; Tuey, G. A. P.
CS Imperial Chem. Industries Ltd., Blackley, Manchester, 9, UK
SO Journal of the Chemical Society (1946) 81-5
CODEN: JCSOA9; ISSN: 0368-1769
DT Journal
LA Unavailable
OS CASREACT 40:17714
AB 2-Amino-4,6-dimethoxypyrimidine (I), b760 252°, m. 92-3°, results in 24-g. yield by heating 32.8 g. of 4,6-dichloro-2-aminopyrimidine (II) with 9.6 g. Na in 160 cc. MeOH and 160 cc. xylene at 140-50° for 3 hrs., distilling the MeOH, adding 100 cc. C6H6 and 200 cc. H2O, filtering, and distilling the C6H6; picrate, yellow, m. 208°. The following homologs were prepared from II and the appropriate alc.: di-EtO (III), b760 265-6°, m. 101° (21.2 g. from 24.6 g. II) (picrate, yellow, m. 162°); di-PrO, b42 184°, m. 72° (16 g. from 16.5 g. II) (picrate, yellow, m. 188°); di(iso-PrO), b30 160°, m. 90° (13.8 g. from 16.5 g. II) (picrate, yellow, m. 108°); di-BuO, b17 192°, m. 58° (27.9 g. from 24.6 g. II) (picrate, yellow, 182-3°); bis(2-ethoxyethoxy), b12 228-30° (24 g. from 16.5 g. II) (picrate, yellow, m. 121°). II (82 g.) and 23 g. Na in 300 cc. MeOH, stirred at room temperature for 24 hrs., give 47 g. of 4-chloro-2-amino-6-methoxypyrimidine (IV), m. 164-6°; 6-EtO homolog (V), m. 87° (6 g. from 16.4 g. (II)). IV (15 g.) with 4.4 g. Na in EtOH and 50 cc. xylene, heated 8 hrs. at 170°, give only 7.7 g. of III; similarly V yielded I. EtONa (2.5 g. Na) in 50 cc. xylene and 17.5 g IV, refluxed 2 hrs., the mixture diluted with C6H6, and extracted with 200 cc. 5 N HCl, give 9.7 g. of 2-amino-4-methoxy-6-ethoxypyrimidine, b736 226-8°, m. 98° (picrate, yellow, m. 185-6°). 4,6-Dichloro-2-amino-5-methylpyrimidine (10.9 g.), heated with MeONa in xylene for 4 hrs. at 160-70°, gives 5 g. of the 4,6-di-MeO derivative, m. 112-14°; the 5-Et homolog m. 92-4°. I (15.5 g.), 23.4 g. p-AcNHC6H4SO2Cl, and 30 cc. C5H5N, heated 1 hr. at 60-70° and 16 hrs. at 40°, give the Ac derivative, m. 235°, of 2-(p-aminophenylsulfonamido)-4,6-dimethoxypyrimidine (VI), m. 171.5° (hydrolysis by boiling with N NaOH for 6 hrs.) (method A); in method B, VI was prepared (in smaller yield) by reacting I with p-O2NC6H4SO2Cl in C5H5N (48 hrs. at 20°) and reducing the crude product with Fe in EtOCH2CH2OH and concentrated HCl. The following homologs were similarly prepared: 4,6-di-EtO (VII), m. 140° (method B; the intermediate NO2 compound m. 156°); di-PrO, m. 128-9° (method B); di(iso-PrO), m. 159-60°; di-BuO (isolated as the Na salt, with 1.5 mols. H2O, m. 275°) (method B; intermediate Na salt (with 1 mol. H2O) of NO2 compound, yellow, m. 140°); 4-methoxy-6-ethoxy, m. 127-8°; 5-Me derivative of VI, m. 227-8°; 5-Et derivative (VIII) of VI, m. 234-6°. 4-Amino-5-phenylpyrimidine and p-O2NC6H4SO2Cl, condensed in C5H5N by heating 2 hrs. on the water bath and the NO2 product reduced with Fe in dilute HCl, give 4-(p-aminophenylsulfonamido)-5-phenylpyrimidine (IX), m. 253-5°, solubility in H2O at 37°, 3.5 mg./100 cc.; the p-anisyl analog m. 269°, and the p-chlorophenyl analog m. 267°. 2-(p-Aminophenylsulfonamido)-4-phenyl-6-methoxypyrimidine (X), m. 236°. 6-(p-Aminophenylsulfonamido)-2-phenyl-4-methylpyrimidine (XI), m. 210-11°. 2-(p-Aminophenylsulfonamido)-4-methoxy-6-methylpyrimidine (XII), m. 167-70°. p-Aminophenylsulfonylguanidine (4.3 g.), 3.4 g. of 1-meth-oxypentane-2,4-dionese, 6 cc. AmOH, and 2 cc.

AcOH heated 16 hrs. at 150°, give 1.1 g. of 2-(p-aminophenylsulfonamido-6-methyl-4-(methoxymethyl)pyrimidine (XIII), m. 167-70°. m-O2NC6H4SO2Cl (11.1 g.), 8.5 g. I, and 50 cc. C5H5N, heated 1 hr. at 90°, give 1.2 g. of 2-(m-aminophenylsulfonamido)-4,6-dimethoxypyrimidine (XIV), m. 134°. I (7.8 g.), 9.3 g. p-O2NC6H4COCl, and 20 cc. C5H5N, mixed at 50-60° and kept at 40° for 16 hrs. and the crude NO2 compound (11.8 g.) reduced with Fe in EtOH-concentrated HCl, give 4.4 g. of 2-(p-aminobenzamido)-4,6-dimethoxypyrimidine (XV), m. 191°. VI exhibited a higher degree of persistence in the blood stream of mice than any other sulfanilamide drug examined; it was also more active in vitro against exptl. streptococcal infections; the Ac derivative was almost as effective in vivo as the free amine (rapid deacetylation in the animal body). Compds. of the type VII and VIII are less effective than VI against infections in mice, although all retain a high degree of persistence in the blood of the exptl. animal but at a lower average level than that given by VI. XIV but not XV behaved similarly to VI, indicating that the sulfonamide group may be essential but that the primary NH2 group need not be in the p-position. Neither XII nor XIII was superior to sulfanilamide in antibacterial activity. Of IX-XI, only I was more effective than sulfanilamide and it was also more persistent in the blood stream of mice than the latter drug.

L5 ANSWER 34 OF 34 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1913:6896 CAPLUS
DN 7:6896
OREF 7:1015d-i,1016a
TI Derivatives of 5-Benzylpyrimidine
AU Kast, Hermann
CS Univ. Berlin
SO Berichte der Deutschen Chemischen Gesellschaft (1913), 45, 3124-35
CODEN: BDCGAS; ISSN: 0365-9496
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. Gerngross, Ber., 38, 3394. 2,4,6-Trichloro-5-benzylpyrimidine (a), from benzylbarbituric acid heated with POCl3 0.5 hr. at 120° in sealed tubes, needles, m. 6.5°, can be distilled only in a high vacuum, easily decompose by alks. Yield, 80-3%. It could not be reduced to benzylpyrimidine by various reagents (Zu dust in b. H2O or in fuming HCl in alc.). With fuming HI containing PH4I, it gives 4-hydroxy-2 (or 6)-iodo-5-benzylpyrimidine (b), needles, m. 208°, soluble in alks. and excess of acids; the I cannot be replaced by NH2 or OH by the action of NH3 or NaOMe. 4-Methoxy-I,6-di-chloro-5-benzylpyrimidine (c), from (a) and NaOMe in MeOH at room temperature prisms, m. 74°, soluble in concentrate HCl, converted by heating with alc. NH3 2 hrs. at 100° into 2-amino-4-methoxy-6-chloro-5-benzylpyrimidine (d), platelets, m. 162°, and by fuming HI into (b) above. 2,4-Dimethoxy-6-chloro-5-benzylpyrimidine, from (a) and 2 mols. NaOMe or from (c) and 1 mol. NaOMe, triclinic rhombohedrons, m. 48°, reduced by Zn dust and fuming HCl in alc. to a yellow oil which, when evaporated to dryness with concentrate HCl, gives 2,4-dihydroxy-5-benzylpyrimidine, prisms, m. 285-6°, also obtained by heating benzyl-barbituric acid with fuming HI and red P 20-5 min. at 150-60°. 2,4,6-Trimethoxy-5-benzylpyrimidine, from (a) and a slight excess of NaOMe at 100°, m. 99.5°. With alc. NH3 at room temperature, (a) gives 2-amino-4,6-dichloro-5-benzylpyrimidine (e), m. 204-5°, and the 4-amino-2,6-dichloro derivative, (f), m. 164°, silky needles from alc., crystals with 0.5 mol. solvent from C6H6. Benzylmalonylguanidine, from PhCH(CO2Et)2, HN: C(NH2)2.HSCN and Na in b. alc., seps. with 1 H2O; heated with POCl3 at 120-5°, it gives (e) in 62-3% yield. (e) is reduced by Zn dust in b. aqueous alc. to 2-amino-5-benzylpyrimidine, scales, m. 133.5° (yield, 25%). Chloroaurate, yellow needles. Chloroplatinate, orange-red needles. With 1 mol. NaOMe in MeOH at 100°, (e) gives (d). (f) with fuming HI yields 4-amino-2(or 6)-iodo-5-benzylpyrimidine, columns, m. 201° (decompose); hydrochloride, rhombohedrons. NH2 cannot be substituted for the I in the base by treatment with alc. NH3 even at 200-10°, but with Zn dust in b. aqueous alc. is obtained the zinc iodide double salt, flat needles, m. about 240°, easily soluble in dilute acids, of 4-amino-5-benzylpyrimidine, platelets, m. 156°. Yield, 65-70%. With alc. NH3 at 150-60°, (a) gives 2,4-diamino-6-chloro-5-benzylpyrimidine (g),needles, m. 163°, also obtained from (e) and alc. NH3 at 160° (yield, 80%), reduced by Zn dust in aqueous alc. HCl at 60-70° to 2,4-diandno-5-benzylpyrimidine, felted needles, m. 145-6°, soluble in hot H2O with alkaline reaction (yield, 8-10%). It is also obtained by treating (g) with fuming HI and PH4I and b. with Zn dust in aqueous alc. HCl the resulting 2,4-diamino-6-iodo-5-benzylpyrimidine, needles, m. 191-2° (turning brown), whose hydroiodide, faintly yellow needles, m. 246-50°, slowly decompose in the air; dis-solves in H2O with acid reaction to litmus.

10/528,959

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	99.17	271.48

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-26.52	-26.52

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